# VEISPH code: two dimensional incompressible SPH code for viscoelastic flows

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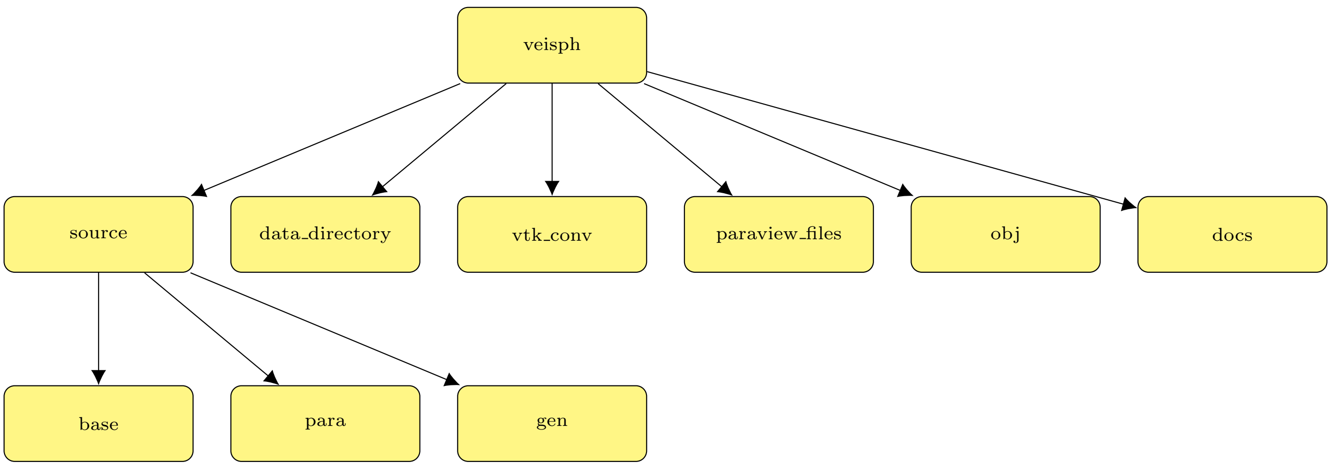
(Dated: March 26, 2021)

A brief description of the VEISPH code. Numerical methods in this code follow arXiv:2009.12245 [1]

## I. DIRECTORY STRUCTURE




- `source` contains source files for the code:
  - `base` contains main modules for VEISPH
  - `para` contains parameters and common variables
  - `gen` contains code to generate casefiles and initial conditions
- `data_directory` contains output files produced by the code
- `vtk_conv` contains a program to convert output files into `.vtu` files, which can be read by Paraview.
- `paraview_files` the program in `vtk_conv` creates `.vtu` files here.
- `obj` contains `.o` and `.mod` files created during compilation.
- `docs` contains this document...

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TABLE I. Strain and relaxation functions for the constitutive models used in this work.

| Constitutive model | $f_S$ | $f_R$ |
|---|---|---|
| Oldroyd B | $\boldsymbol{A}-\boldsymbol{I}$ | $\boldsymbol{A}-\boldsymbol{I}$ |
| FENE-P | $\frac{\boldsymbol{A}}{1-tr(\boldsymbol{A})/L^2}-\boldsymbol{I}$ | $\frac{\boldsymbol{A}}{1-tr(\boldsymbol{A})/L^2}-\boldsymbol{I}$ |
| FENE-CR | $\frac{\boldsymbol{A}-\boldsymbol{I}}{1-tr(\boldsymbol{A})/L^2}$ | $\frac{\boldsymbol{A}-\boldsymbol{I}}{1-tr(\boldsymbol{A})/L^2}$ |
| Linear PTT | $\boldsymbol{A}-\boldsymbol{I}$ | $\left[1+\varepsilon tr\left(\boldsymbol{A}-\boldsymbol{I}\right)\right]\left(\boldsymbol{A}-\boldsymbol{I}\right)$ |
| Exponential PTT | $\boldsymbol{A}-\boldsymbol{I}$ | $\exp\left[\varepsilon tr\left(\boldsymbol{A}-\boldsymbol{I}\right)\right]\left(\boldsymbol{A}-\boldsymbol{I}\right)$ |
| Giesekus | $\boldsymbol{A}-\boldsymbol{I}$ | $\alpha\boldsymbol{A}^2+\left(1-2\alpha\right)\boldsymbol{A}-\left(1-\alpha\right)\boldsymbol{I}$ |

## II. GOVERNING EQUATIONS

The governing equations (here listed in dimensionless form) in the arbitrary frame of reference as in [1] are:

$$\nabla\cdot\boldsymbol{u}=0 \tag{1a}$$

$$\frac{d\boldsymbol{u}}{dt}-\boldsymbol{u_s}\cdot\nabla\cdot\boldsymbol{u}=-\nabla p+\beta\sqrt{\frac{Pr}{Ra}}\nabla^2\boldsymbol{u}+\frac{\left(1-\beta\right)Pr}{Ra\times El}\nabla\cdot\boldsymbol{\tau_p}+\theta\boldsymbol{e_y}+\boldsymbol{f} \tag{1b}$$

$$\frac{d\boldsymbol{A}}{dt}-\boldsymbol{u_s}\cdot\nabla\boldsymbol{A}-\left(\boldsymbol{A}\cdot\nabla\boldsymbol{u}^T+\nabla\boldsymbol{u}\cdot\boldsymbol{A}\right)=\frac{-1}{El}\sqrt{\frac{Pr}{Ra}}f_R\left(\boldsymbol{A}\right) \tag{1c}$$

$$\frac{d\theta}{dt}-\boldsymbol{u_s}\cdot\nabla\theta=\frac{1}{\sqrt{Ra\times Pr}}\nabla^2\theta \tag{1d}$$

where $\boldsymbol{u}$ is the velocity, $p$ the pressure, $\theta$ the temperature deviation (from ambient), and $\boldsymbol{\tau_p}$ is the polymeric stress, related to the conformation tensor $\boldsymbol{A}$ by the strain function $\boldsymbol{\tau_p}=f_S\left(\boldsymbol{A}\right)$. $f_R$ is a relaxation function. $\boldsymbol{f}$ is a body force.

*N.B. Equation* (1d) *is not yet implemented in the code!*

The system is controlled by the four dimensionless quantities:

$$\beta=\eta_s/\eta_0 \qquad \text{Viscosity ratio} \tag{2a}$$

$$Pr=\frac{c_p\eta_0}{\kappa} \qquad \text{Prandtl number} \tag{2b}$$

$$Ra=\frac{L^3\Delta\rho\left|\boldsymbol{g}\right|}{\alpha\eta_0} \qquad \text{Rayleigh number} \tag{2c}$$

$$El=\frac{\lambda\eta_0}{L^2} \qquad \text{Elasticity number,} \tag{2d}$$

where $\eta_s$ is the solvent viscosity, $\eta_0$ is the total viscosity, $c_p$ is the specific heat capacity (at const. pressure), $\kappa$ is the thermal diffusivity, $\alpha$ is the thermal conductivity (related to $\kappa$ via density $\rho$ and $c_p$), $\boldsymbol{g}$ is the acceleration due to gravity, $\Delta\rho$ is a characteristic density deviation, $\lambda$ is the relaxation time and $L$ is a characteristic length-scale.

The Reynolds number is related to these dimensionless groups by: $Re=\sqrt{Ra/Pr}$. The Weissenberg number is $Wi=El\sqrt{Ra/Pr}$.

The strain and relaxation functions for various constitutive models are given in Table I.

Time evolution is with a first-order projection scheme [2], with divergence free velocity constraint enforced via a Poisson equation, which is solved using a BiCGStab algorithm with Jacobi preconditioner. Boundary conditions are imposed with mirror particles. SPH gradient and divergence operators are corrected to first order following [3]. Temporal evolution of the conformation tensor is via the log-conformation formulation of [4, 5], mostly following [6].

## III. ELASTO-VISCOUS STRESS SPLITTING

With the above non-dimensionalisation, we introduce the tensor

$$\boldsymbol{\Phi}=\boldsymbol{\tau_p}-\frac{\alpha_{evss}El}{1-\beta}\sqrt{\frac{Ra}{Pr}}\left(\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^T\right) \tag{3}$$

and then express (1b) as

$$\frac{d\boldsymbol{u}}{dt}-\boldsymbol{u_s}\cdot\nabla\cdot\boldsymbol{u}=-\nabla p+(\beta+\alpha_{evss})\sqrt{\frac{Pr}{Ra}}\nabla^2\boldsymbol{u}+\frac{(1-\beta)\,Pr}{Ra\times El}\nabla\cdot\boldsymbol{\Phi}+\theta\boldsymbol{e_y}+\boldsymbol{f}. \tag{4}$$

This formulation introduces a small amount of additional viscosity into the solvent part, and then removes the same amount via the divergence of $\boldsymbol{\Phi}$, improving stability when $\beta$ is small or zero. For $\beta>0.1$ we can usually set $\alpha_{evss}=0$, and (4) returns to (1b). For smaller $\beta$, values of $\alpha_{evss}$ between 0.01 and 0.1 are usually sufficient to provide stability.

## IV. BOUNDARY FRAMEWORK

The computational domain is described by a set of boundary nodes, connected by straight lines (boundary patches), along with circles. In `datclass.F90` these are hard-coded for each case. For example, a rectangular domain with solid upper and lower boundaries and periodic lateral boundaries would be defined as:

```
b_type(:) = (/ 1, 2, 1, 2/)
b_vel(:) = (/ -0.0d0,0.0d0,0.0d0,0.0d0/)
b_periodic_parent(:) = (/ 3, 4, 1, 2/)
b_node(1,:) = (/ 0.0d0, 0.0d0 /)
b_node(2,:) = (/ xl, 0.0d0 /)
b_node(3,:) = (/ xl, yl /)
b_node(4,:) = (/ 0.0d0, yl /)
```

where `xl` and `yl` are variables describing the length and height of the domain. The array `b_vel` indicates the velocity (tangential to the boundary patch) and here is usually zero. The array `b_type` indicates whether the patch is a wall (1) periodic (2), invisible (0) or (in other versions, but not relevant to this project) inflow (3) or outflow (4). For periodic patches, a relationship needs to be defined with a parent patch, which is done via the array `b_periodic_parent`.

Circular obstacles are described similarly, with centre `c_centre`, radius `c_radius`, angular velocity `c_omega` and translational velocity `c_vel`. In this project, the translational velocities will probably always be zero. A positive value of `c_radius` indicates the circle is an internal obstacle (e.g. the inner boundary in Taylor-Couette flow), whilst a negative value indicates the circle is an external boundary (e.g. the outer boundary in Taylor-Couette flow).

### A. How boundary conditions are applied in the code

In the code (`source/base/mirror_boundaries_mod.F90`), the routine runs through all particles and identifies those near boundaries. Then, it runs through each boundary, and for all particles near that boundary, creates a mirror particle in the appropriate place, with appropriate conditions. The code then runs through all corners (i.e. all boundary nodes), and performs a similar procedure. Each mirror particle $j$ has a parent particle $i$, and the array `irelation` tracks this: `irelation(j)=i`. The array `vrelation` stores information (in a confusing way) about the type of boundary which relates a mirror and its parent, and is used in specifying velocity relationships.

For example, if particle $i$ is near a solid boundary patch, a particle $j$ will be created which is a reflection of particle $i$ in the boundary patch. Particle $j$ will have velocity $\boldsymbol{u}_j=2\boldsymbol{u}_b-\boldsymbol{u}_i$, where $\boldsymbol{u}_b$ is the velocity of the boundary patch.

Pressure boundary conditions ($\boldsymbol{n}\cdot\nabla p=\boldsymbol{f}\cdot\boldsymbol{n}$) are constructed by specifying the difference between a mirror and its parent pressure through the array `dp_mp`, such that `P(i) = P(j) + dP_mp(i)`.

## V. OVERVIEW OF THE CODE STRUCTURE

The code consists of modules, each module is stored in a separate `.F90` file. Each module contains one or more subroutines which perform similar tasks, or tasks related to a theme (e.g. the module `part_shift` contains routines related to Fickian shifting).

The main program is contained within `sph2D_incom.F90`. It calls routines from the input module `input.F90`, some other housekeeping, then contains the main time loop. Within the main time loop, the routine `div_free` is called, which performs a single time step, then `output` is called, which saves any data as required. The module `div_free.F90` is the heart of the code, and is fairly clearly commented, the the subroutine `divfree` corresponds (roughly) to the steps 1 to 7 on pages 5 and 6 of [1].

# VI. CASE CREATION, COMPILING, RUNNING AND POSTPROCESSING

## A. Case creation

In the directory `source/gen/` there is a file `datclass.F90`. This is the main part of a program which generates the input data for the code. Navigate to this directory, and then build and run it with:

```
make
./gen2D
cp I* ../../.
```

When you run `./gen2D`, it will give a list of cases and prompt you to choose one. Type the relevant number and press enter. You can modify `datclass.F90` to create more cases.

The following cases are currently included in `datclass.F90`:

1. 2D dam break
2. Taylor Green vortices
3. Poiseuille flow
4. Taylor-Couette flow
5. Periodic cylinders in a channel (as in [7])
6. Kolmogorov flow (you need to set the `external_forcing` switch to `.true.`).
7. Plane Couette flow

## B. Compiling and running the code

The Makefile is built for systems with the compiler `gfortran` install. If using an alternative compiler, modify the lines `FC := gfortran` and `LD := gfortran` to point to your chosen compiler. You need a system with OpenMP installed.

To compile and run the code,

1. Navigate the main directory `veisph`
2. Compile the code with the command `make const_mod=X`, where `X` points to the constitutive model of you want. 1 gives Newtonian, 2 to 7 give Oldroyd B, FENE-P, FENE-CR, Linear PTT, Exponential PTT and Giesekus (respectively). Oldroyd B is the simplest viscoelastic constitutive model, and first to experiment with.
3. Run the code by typing `./veisph`

# VII. POST-PROCESSING

Data from the code are saved in the folder `data_directory`. Within the folder `vtk_conv` there is a small program which converts the data into a format which can be read by Paraview.

To process the results

1. Navigate in a terminal to `vtk_conv`
2. Run `./a.out`
3. The files which paraview can read will be created in the folder `paraview_files`

To view the files, open paraview, and open the files `PART00XX`.

Additional outputs/diagnostics are saved as files called `fort.XXX`. For example, a routine in `div_free.F90` writes the maximum velocity in the domain at each output time to the file `fort.192`.

## VIII. LINUX TIPS

- Use tab key to autocomplete;
- `cd ../` navigates up one level;
- Similarly, `cp x ../.` copies file `x` up one level;
- Use up/down arrow keys to scroll through command line history;
- Ctrl+shift+N opens a new terminal;
- In a file browser, you right click–¿ open in terminal;
- Ctrl+C aborts a program.

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